A Consistent X-ray Photoabsorption Spectrum for Interstellar Atomic Gas and Silicate Dust

Completed Technology Project (2017 - 2019)

Project Introduction

This proposal sets out to answer the following astrophysically important questions: Where are oxygen, silicon, and iron found in the universe? What are their abundances and physical and chemical forms? A complete set of atomic, molecular, and solid-state photoabsorption data. We propose to generate such data through a combination of the following theoretical techniques. Firstly, R-matrix calculations will be carried out to obtain the K-shell photoabsorption of atomic silicon and the L-shell of iron; in this respect atomic oxygen has already been extensively treated by us. Secondly, the UK molecular R-matrix (UKRmol) package will be used to compute the photoabsorption of molecular oxygen (O_2), carbon monoxide (CO), carbon dioxide (CO_2). And thirdly, we will implement multiple scattering theory in tandem with an atomic R-matrix treatment for each atom to compute photoabsorption cross sections for condensed-matter systems such as oxides, silicates, and other compounds comprising interstellar dust and ice. A final model will be developed in a fashion consistent with the photoabsorption in all environments - atomic, molecular, and solid-state. To this end, a consistent model for all cases is developed that (1) preserves the oscillator strength sum rule per electron, and (2) exhibits the expected identical absorption away from the inner-shell thresholds. Such a model allows for a controlled measure of the quantitative differences in the near-edge structure of atomic, molecular, and solid-state X-ray spectral observations. For oxygen, the atomic neutral and ionic cross sections are now well established from our recent work, and we will use the UKRmol codes to compute K-shell photoabsorption cross sections for O_2, CO, and H_2O. For more complicated systems, we will perform R-matrix calculations for the individual atoms and utilize multiple scattering theory to compute the photoabsorption cross section. For Si, atomic R-matrix calculations will be performed for the K-shell atomic cross sections, and then multiple scattering theory will be used to treat more complex systems. For the more complex case of iron L-shell absorption, we will perform large-scale atomic R-matrix calculations, using three approaches: a non-relativistic LS-coupled Hamiltonian, a Breit-Pauli Hamiltonian, and a Dirac-Fock Hamiltonian, the latter two to include the important fine-structure splitting of thresholds. Multiple scattering theory will be used with the atomic R-matrix information to treat photoabsorption in solid-state environments, and a consistent atomic, molecular, and solid-state absorption model will be developed. By determining atomic, molecular and solid state cross sections on the same footing, we will use available experimental and astronomical (Chandra) observations, in the case of atomic oxygen, and experimental cross sections, in the case of silicates, to calibrate the exact position of all K-shell thresholds, as well as the absolute cross sections. Moreover, current experimental cross sections for a few silicate compositions will help us study the effects of chemical binding on the position and shape of the cross sections across inner-shell thresholds. Thus, we will be able to provide self-consistent cross sections for all forms of oxygen, silicon, and iron in the X-ray region accessible to Chandra and XMM-Newton. The derived data and analytical model will be made available to the

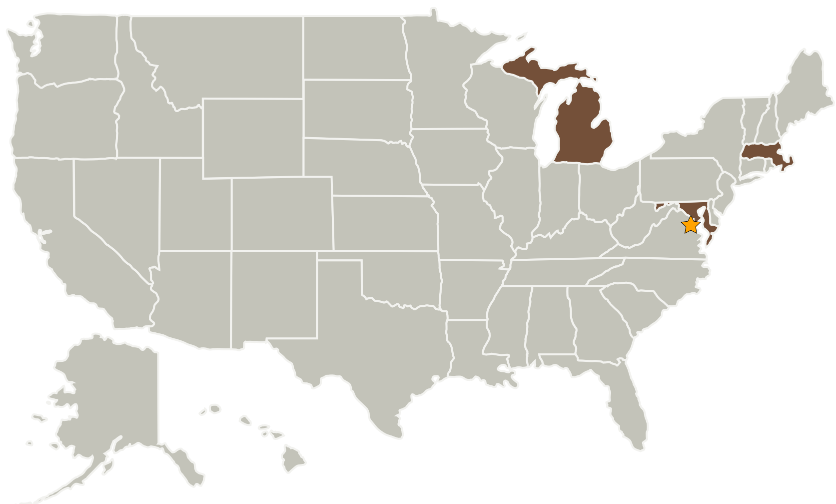
Image Not Available

A Consistent X-ray Photoabsorption Spectrum for Interstellar Atomic Gas and Silicate Dust

Table of Contents

astrophysics community, and will be incorporated into the XSTAR database for x-ray spectral modeling analysis. From observed x-ray spectra near the K-edge of O and Si, and the L-edge of Fe, we will infer the compositions of each of these three elements and help answer the question posed initially: in what forms and abundances are oxygen, silicon, and iron found in the universe?

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
★NASA Headquarters(HQ)	Lead Organization	NASA Center	Washington, District of Columbia

Primary U.S. Work Locations	
Maryland	Massachusetts
Michigan	

Organizational Responsibility

Responsible Mission Directorate:

Science Mission Directorate (SMD)

Lead Center / Facility:

NASA Headquarters (HQ)

Responsible Program:

Astrophysics Research and Analysis

Project Management

Program Director:

Michael A Garcia

Program Manager:

Dominic J Benford

Principal Investigator:

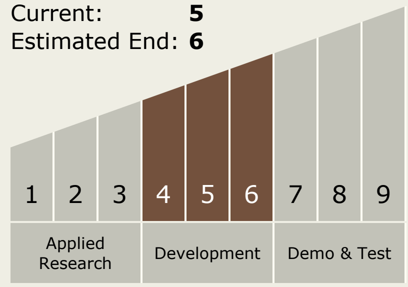
Thomas W Gorczyca

Co-Investigators:

Sarah D Pratt
Javier A Garcia
Timothy Kallman
Manuel A Bautista-plaza

Technology Maturity (TRL)

Start: **4**
Current: **5**
Estimated End: **6**



Technology Areas

Primary:

- TX02 Flight Computing and Avionics
  - └ TX02.1 Avionics Component Technologies
    - └ TX02.1.3 High Performance Processors

Target Destination

Outside the Solar System